# Bose-Einstein Condensation of Confined and Non-interacting Bose Particles by the Integral Representation of Bose Functions

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With the integral representation of Bose functions, the Bose-Einstein condensation of non-interacting bosons in a three-dimensional harmonic trap was studied. The relation between the particle number and its phase transition temperature was clarified. Some next-order terms in the thermodynamic expansions were obtained. We plotted the chemical potential, the mean energy, and the specific heat and found most of these properties obtained by using the integral representation were almost identical with those of the series representation of Bose functions.

After the historical paper by Bose and Einstein in the 1920s, the observation of a Bose-Einstein condensation (BEC) was successfully demonstrated in magneto-optical traps (MOT) of dilute alkali gases about a decade ago [1, 2]. Although the Bose atoms in the MOT are confined and interacting [3, 4, 5], a confined and non-interacting Bose system was studied because it is analytic and gives some clue for the lab system when the number of particles is not very large. However, the previous studies have been based on series representations of the Bose functions [6, 7, 8, 9].

In this paper, we study a very fundamental part of the BEC of confined and non-interacting Bose particles by using an integral representation of the Bose functions [10]. We obtain the relation between the number of particles and the shift of $T_c$, the temperature of the phase transition, exactly. The chemical potential and the specific heat around $T_c$ will be displayed to find the phase transition. In principle, we will follow the method introduced by Haugerud *et al.* during the statistical analysis [8, 9].

Consider a 3D system of $N$ non-interacting bosons confined by a harmonic potential of angular frequency $\omega$. The discrete one-body energy eigenvalues of the harmonic oscillator potential are given by $\varepsilon_n = \hbar(n_x\omega_x + n_y\omega_y + n_z\omega_z) + \varepsilon_0$, where $n_x, n_y, n_z = 0, 1, 2, ...$ and $n = \{n_x, n_y, n_z\}$. The zero-point energy is given by $\varepsilon_0 = (1/2)\hbar(\omega_x + \omega_y + \omega_z)$. The distribution function of bosons in the grand canonical ensemble at temperature $T$ is given by

$$N = \sum_{n_x, n_y, n_z} \frac{1}{e^{\beta(\varepsilon_n - \mu)} - 1}, \tag{1}$$

where $\beta = 1/k_B T$, $k_B$ is the Boltzmann constant, and $\mu$ is the chemical potential. For simplicity, we here ignore the anisotropy of the trap and consider a typical trap potential of $\omega_x = \omega_y = \omega_z = \omega = 10^3 sec^{-1}$. Since each energy level has a degeneracy $d(n) = (n+1)(n+2)/2$, the total number $N$ in Eq. (1) is written as

$$
\begin{aligned}
N &= \frac{1}{e^{\beta(\varepsilon_0 - \mu)} - 1} + \sum_{n=1}^{\infty} \frac{d(n)}{e^{\beta(\varepsilon_n - \mu)} - 1} \\
&= \frac{1}{z^{-1}e^{\beta\varepsilon_0} - 1} + \sum_{m=0}^{\infty} \frac{\frac{1}{2}m^2 + \frac{5}{2}m + 3}{e^{-\beta\mu + \beta\hbar\omega + \beta\hbar\omega m} - 1}, \\
&\equiv N_0 + N_e, 
\end{aligned}
\tag{2}
$$

where $z = e^{\beta\mu}$ is the fugacity.

There are various ways to convert the summation into integrals, and here we use the Euler-Maclaurin's summation-integral formula [7, 8, 9, 11]. Then, the $N$ in Eq. (2) turns into the following integral forms:

$$
\begin{aligned}
N &= N_0 + \frac{1}{(\beta\hbar\omega)^3}F_3(\alpha) + \frac{5}{2(\beta\hbar\omega)^2}F_2(\alpha) \\
&\quad + \frac{3}{\beta\hbar\omega}F_1(\alpha) + \frac{31}{24}\frac{1}{e^\alpha - 1} + \frac{\beta\hbar\omega}{4}\frac{e^\alpha}{(e^\alpha - 1)^2},
\end{aligned}
\tag{3}
$$

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where $\alpha = -\beta\mu + \beta\hbar\omega$, $e^{-\alpha} = e^{\beta(\mu - \hbar\omega)} = z_e$ is the effective fugacity [8, 9], and $F_s(\alpha)$ is the integral representaion of Bose functions defined by [10]

$$F_s(\alpha) \equiv \frac{1}{\Gamma(s)} \int_0^\infty \frac{x^{s-1}}{e^{\alpha+x} - 1} dx, \tag{4}$$

with $s > 0$. $F_s$ is related to the series representation of Bose functions, $g_s(z) = \sum_{n=1}^\infty z^n/n^s$, by way of the effective fugacity as $F_s(\alpha) = g_s(z_e)$.

The Riemann-zeta function is a special case of the integral as $F_s(0) = g_s(1) = \zeta(s)$, and there are several more useful properties [11]:

$$\frac{dF_s(\alpha)}{d\alpha} = -F_{s-1}(\alpha), \tag{5}$$

where $s > 1$. Note that $dg_s(z)/dz = g_{s-1}(z)/z$. When $\alpha$ is small, $F_s(\alpha)$ can be expanded by using a power series of the $\alpha$ as [10]

$$\begin{aligned} F_s(\alpha) &= \Gamma(1-s)\alpha^{s-1} + \sum_{n=0}^\infty \zeta(s-n)\alpha^n \\ &\simeq \Gamma(1-s)\alpha^{s-1} + \zeta(s) + \dots \end{aligned} \tag{6}$$

For the first two values of the integer $s$, $F_s(\alpha)$ is given by

$$\begin{aligned} F_2(\alpha) &= \zeta(2) - \alpha(1 - \ln\alpha) + \dots , \tag{7} \\ F_1(\alpha) &= -\ln\alpha + \dots \tag{8} \end{aligned}$$

Since $\beta\hbar\omega \ll 1$, $N_e$ in Eq. (3) is expanded around $-\beta\mu$ with the help of Eq. (5) as

$$\begin{aligned} N_e &= \frac{1}{(\beta\hbar\omega)^3}\left[F_3(-\beta\mu) + F_3'(-\beta\mu)\beta\hbar\omega + \frac{1}{2!}F_3''(-\beta\mu)(\beta\hbar\omega)^2\right] \\ &\quad + \frac{5}{2(\beta\hbar\omega)^2}\left[F_2(-\beta\mu) + F_2'(-\beta\mu)\beta\hbar\omega\right] + \frac{3}{\beta\hbar\omega}F_1(-\beta\mu) \\ &\quad + \frac{31}{24}\frac{1}{e^{-\beta\mu} - 1} + \frac{1}{4}\frac{\beta\hbar\omega e^{-\beta\mu}}{(e^{-\beta\mu} - 1)^2} + \dots \\ &= \frac{1}{(\beta\hbar\omega)^3}F_3(-\beta\mu) + \frac{3}{2(\beta\hbar\omega)^2}F_2(-\beta\mu) + \mathcal{O}\left(\frac{1}{\beta\hbar\omega}\right). \end{aligned} \tag{9}$$

Substituting Eq. (9) into Eq. (2), we find that the number of particles in the condensate varies with the temperature as [6, 7, 8, 9]

$$N_0 = N - \left(\frac{k_B T}{\hbar\omega}\right)^3 F_3(-\beta\mu) - \frac{3}{2}\left(\frac{k_B T}{\hbar\omega}\right)^2 F_2(-\beta\mu). \tag{10}$$

In the transition region, $\mu \to 0$, then, $F_s$ becomes the Riemann-zeta function $\zeta(s)$.

Defining the transition temperature $T_c$ where $N_0 = 0$ in Eq. (10), we find that

$$\begin{aligned} T_c &= \frac{\hbar\omega}{k_B}\left(\frac{N}{\zeta(3)}\right)^{1/3}\left[1 - \frac{3\zeta(2)}{2N}\left(\frac{k_B T_c}{\hbar\omega}\right)^2\right]^{1/3} \\ &= T_0\left[1 - \frac{A}{2}(1 - A + A^2 - A^3 + \dots)\right] \\ &= T_0\left[1 - \frac{A}{2(1+A)}\right], \end{aligned} \tag{11}$$

where

$$T_0 = \frac{\hbar\omega}{k_B}\left(\frac{N}{\zeta(3)}\right)^{1/3}. \tag{12}$$

This is the microcanonical critical temperature for the infinite system. $A$ in Eq. (11) is the one-dimensional inverse particle number defined by

$$A(N) \equiv \frac{\zeta(2)}{\zeta(3)^{2/3} N^{1/3}} = \frac{1.455}{N^{1/3}}. \tag{13}$$

Therefore, the ratio of the shift of $T_c$ is given by [6]

$$S(N) = \frac{T_0 - T_c}{T_0} = \frac{A}{2(1+A)}. \tag{14}$$

If $N \leq 198$, then the $S(N)$ is more than 10%. Similarly, $N = 2000$ corresponds to about 5% and $N = 20000$ to about 2.5%. We plotted the $S(N)$ as a function of $N$ in Fig. 1. Since $S(N) \to 0$ for large $N$, $T_0$ will be a useful standard temperature for discussion. Therefore, Eq. (10) is written with the definition of $T_0$ as [8, 9]

$$\frac{N_0}{N} = 1 - \left(\frac{T}{T_0}\right)^3 \frac{F_3(-\beta\mu)}{\zeta(3)} - \frac{3}{2}\left(\frac{T}{T_0}\right)^2 \frac{F_2(-\beta\mu)}{\zeta(3)^{2/3} N^{1/3}}. \tag{15}$$

The condensate fraction is plotted in Fig. 2 for increasing $N$ The sudden flattening of the curves takes place around $T_c$.

The negative shift [6] in Eq. (11) is expanded up to the order of $N^{-2/3}$ as

$$\begin{aligned} \frac{T_c - T_0}{T_0} &= -\frac{A}{2(1+A)} \\ &= -\frac{0.7275}{N^{1/3}} + \frac{1.059}{N^{2/3}} + \ldots \end{aligned} \tag{16}$$

The chemical potential for $N = 200$, $N = 2000$, and $N = 20000$ is plotted in Fig. 3. It approaches 0 as $T \to T_c$. Note that there is a cross at $T = T_0$.

The specific heat is obtained from the first derivative of its mean energy. The mean energy of the system is the internal energy of $N$ non-interacting and harmonically confined bosons:

$$U = \sum_{n=0}^{\infty} \frac{d(n)\varepsilon_n}{e^{\beta(\varepsilon_n - \mu)} - 1}. \tag{17}$$

The zero-point mean energy is small in the condensate state. If we apply the Euler-Maclaurin formula Eq. (17), we can write $U(T)$ in the similar way with Eq. (9) as

$$\begin{aligned} \frac{U}{\hbar\omega} &= \frac{N\varepsilon_0}{\hbar\omega} + \sum_{m=0}^{\infty} \frac{\frac{1}{2}m^3 + 3m^2 + \frac{11}{2}m + 3}{e^{\alpha + \beta\hbar\omega m - \mu} - 1} \tag{18} \\ &= \frac{U_0}{\hbar\omega} + \frac{3}{(\beta\hbar\omega)^4} F_4(\alpha) + \frac{6}{(\beta\hbar\omega)^3} F_3(\alpha) + \frac{11}{2(\beta\hbar\omega)^2} F_2(\alpha) \\ &\quad + \frac{3}{\beta\hbar\omega} F_1(\alpha) + \frac{25}{24} \frac{1}{e^\alpha - 1} + \frac{\beta\hbar\omega}{4} \frac{e^\alpha}{(e^\alpha - 1)^2} + \ldots \tag{19} \end{aligned}$$

We may expand $U$ around $\alpha = -\beta\mu$. Then, we have

$$\frac{U}{\hbar\omega} = \frac{U_0}{\hbar\omega} + \frac{3}{(\beta\hbar\omega)^4} F_4(-\beta\mu) + \frac{3}{(\beta\hbar\omega)^3} F_3(-\beta\mu) + \frac{1}{(\beta\hbar\omega)^2} F_2(-\beta\mu) + \ldots \tag{20}$$

Note that the $F_1$ term does not exist here. Replacing $k_B/\hbar\omega$ with $T_0$ in Eq. (12), we obtain the energy per particle as a function of $T/T_0$:

$$\frac{U - U_0}{N\hbar\omega} = 3\left(\frac{T}{T_0}\right)^4 \frac{F_4(-\beta\mu)}{\zeta(3)^{4/3} N^{-1/3}} + 3\left(\frac{T}{T_0}\right)^3 \frac{F_3(-\beta\mu)}{\zeta(3)} + \left(\frac{T}{T_0}\right)^2 \frac{F_2(-\beta\mu)}{\zeta(3)^{2/3} N^{1/3}}. \tag{21}$$

We plotted $(U - U_0)/N\hbar\omega$ of Eq. (21) in Fig. 4. The phase transition is shown at $T_c$.

If we take the partial derivatives with respect to temperature in Eq. (20), the specific heat around $T_c$ is obtained for two ranges:

(i) When $T \leq T_c$,

$$\frac{C_V^-}{Nk_B} = 12 \left(\frac{T}{T_0}\right)^3 \frac{F_4(-\beta\mu)}{\zeta(3)} + 9 \left(\frac{T}{T_0}\right)^2 \frac{F_3(-\beta\mu)}{\zeta(3)^{2/3} N^{1/3}}. \tag{22}$$

(ii) When $T > T_c$,

$$\begin{aligned}
\frac{C_V^+}{Nk_B} &= 12 \left(\frac{T}{T_0}\right)^3 \frac{F_4(-\beta\mu)}{\zeta(3)} + 9 \left(\frac{T}{T_0}\right)^2 \frac{F_3(-\beta\mu)}{\zeta(3)^{2/3} N^{1/3}} \\
&\quad - 3T_0 \left[ \left(\frac{T}{T_0}\right)^4 \frac{F_3(-\beta\mu)}{\zeta(3)} + \left(\frac{T}{T_0}\right)^3 \frac{F_2(-\beta\mu)}{\zeta(3)^{2/3} N^{1/3}} \right] \frac{\partial \alpha}{\partial T}.
\end{aligned} \tag{23}$$

The $\partial\alpha/\partial T$ is obtained from Eq. (12) as

$$\frac{\partial \alpha}{\partial T} = \frac{3}{T} \frac{F_3(-\beta\mu) + \frac{T_0}{T} \left(\frac{\zeta(3)}{N}\right)^{1/3} F_2(-\beta\mu)}{F_2(-\beta\mu) + \frac{3T_0}{2T} \left(\frac{\zeta(3)}{N}\right)^{1/3} F_1(-\beta\mu)}. \tag{24}$$

When $\mu$ approaches zero, $\partial\alpha/\partial T$ in Eq. (24) becomes zero, too, because $F_1$ diverges. Therefore, $C_V^-$ in Eq. (22) and $C_V^+$ in Eq. (23) match at $T_c$. The basic procedure is the same as shown in Ref. [6].

$C_V/Nk_B$ is plotted in Fig. 5. The specific heat exhibits a sharp jump like the $\lambda$ transition. Since the divergence of $F_1$ is extremely slow, it is very difficult to find the continuity at $T_c$ in the numerical calculation, but the sudden drop of $C_V$ in the vicinity of $T_c$ is clear. As previous research pointed out [6, 8, 9], the $\lambda$-like phase transition in the specific heat is seen for any small number of non-interacting and confined bosons.

The discontinuity of the specific heat at $T_0$ was obtained as a function of $N$. If we expand this equation up to terms of $1/N^{1/3}$, we obtain the following form:

$$\frac{C_V^+}{Nk_B} = 12 \left(\frac{T}{T_0}\right)^3 \frac{F_4(-\beta\mu)}{\zeta(3)} - 9 \left(\frac{T}{T_0}\right)^3 \frac{F_3(-\beta\mu)^2}{\zeta(3)F_2(-\beta\mu)}. \tag{25}$$

Except the $T_c$, the point of sudden drop of the slops, the divergence of $F_1(-\beta\mu)$ is extremely slow. Therefore, at $T > T_c$, the $N^{1/3}$ dominantes $F_1$ and the approximation is obtained as

$$\begin{aligned}
\frac{C_V^- - C_V^+}{Nk_B} &= 9 \frac{\zeta(3)}{\zeta(2)} + 9 \left(\frac{\zeta(3)}{N}\right)^{1/3} \\
&= 6.577 + \frac{9.569}{N^{1/3}}.
\end{aligned} \tag{26}$$

If $N$ is order of $10^3$, the second term is about 10% of the first term.

We rewrote the BEC of confined and non-interacting Bose particles in 3D by using the integral representation of Bose functions. We obtained the exact relation between the number of particles and the shift of $T_c$ and showed how the thermodynamic limit of the condensate fraction is achieved around $T_c$ with increasing $N$. The chemical potential around $T_c$ was plotted for increasing $N$. It has a common point at $T_0$, regardless of the number of particles. We plotted the mean energy and the specific heat around $T_c$. Although we used the integral representation of the Bose functions, we see that the results are almost identical with previous results obtained by using a series representation of Bose functions.

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[1] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Weimann, and E. A. Cornell, Science **269**, 198 (1995).
[2] K. B. Davis, H.-O. Mewes, M. R. Andrews, N. J. van Druten, D. S. Durfree, D. M. Kurn, and W. Ketterle, Phys. Rev. Lett. **75**, 3969 (1995).
[3] S.-H. Kim, S. D. Oh, and W. Jhe, J. Korean Phys. Soc. **37**, 665 (2000).

[4] D. Kim, G. Jin, and J.-H. Yoon J. Korean Phys. Soc. **46**, 1336 (2005).

[5] S.-H. Kim and C. S. Kim, J. Korean Phys. Soc. **48**, 158 (2006).

[6] S. Grossmann and M. Holthaus, Phys. Lett. A **208**, 188 (1995).

[7] W. J. Mullin, J. Low Temp. Phys. **106**, 615 (1997).

[8] H. Haugerud, T. Haugset, and F. Ravndal, Phys. Lett. A **225**, 18 (1997).

[9] T. Haugset, H. Haugerud, and J. O. Anderson, Phys. Rev. A **55**, 2922 (1997).

[10] J. E. Robinson, Phys. Rev. **83**, 678 (1951).

[11] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1972).
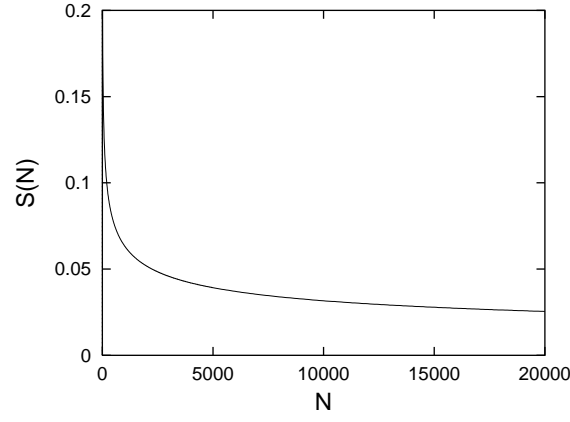
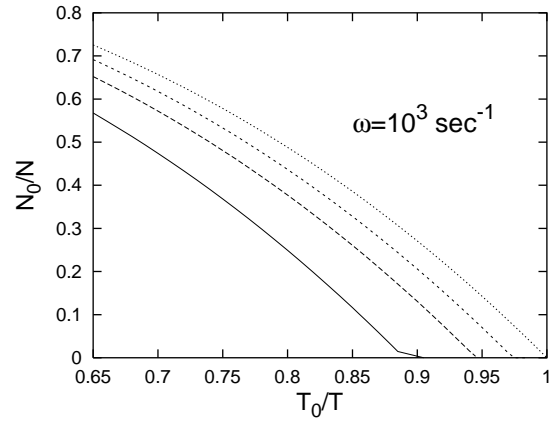FIG. 1: Ratio of the shift of the phase transition temperature as a function of $N$.



FIG. 2: Condensate fraction around $T_c$. The solid line is for $N = 200$, the long-dashed line is for $N = 2000$, the short-dashed line is for $N = 20000$, and the dotted line is for the $N \rightarrow \infty$ limit.
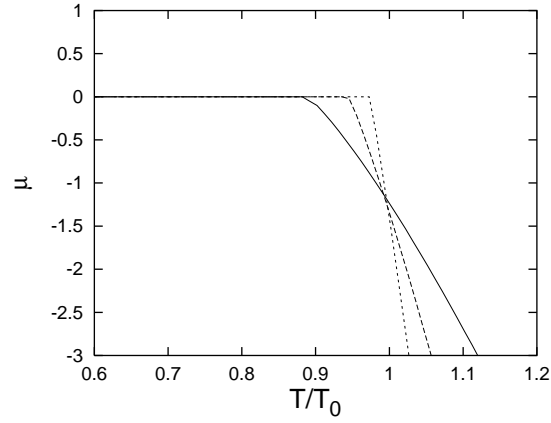


FIG. 3: Chemical potential around $T_c$. The solid line is for $N = 200$, the long-dashed line is for $N = 2000$, and the short-dashed line is for $N = 20000$.
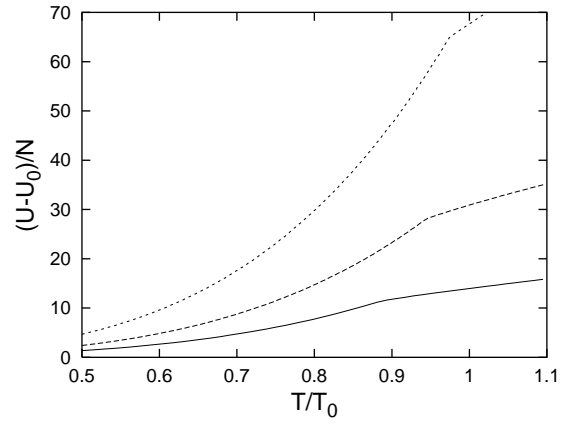
FIG. 4: Mean energy around $T_c$. The unit is $\hbar\omega$. The solid line is for $N = 200$, the long-dashed line is for $N = 2000$, and the short-dashed line is for $N = 20000$.
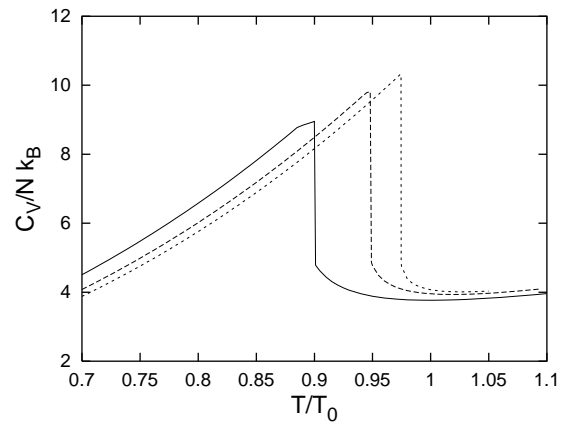


FIG. 5: Specific heat around $T_c$. From left to right, $N = 200$, $N = 2000$, and $N = 20000$.